

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Data Requirement: PMRA Data Code: 8.2.3.2
EPA DP Barcode: 349858
OECD Data Point: IIA 2.9.1
EPA Guideline: 835.2120

Test material:

Common name: Saflufenacil.

Chemical name:

IUPAC name: N'-(2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl)-N-isopropyl-N-methylsulfamide.
N'-(2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl)-N-isopropyl-N-methylsulfamide.

CAS name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS No.: 372137-35-4.

Synonyms: BAS 800 H, CL No. 433379, 4054449, AC 433,379.

Smiles string: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

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June 8, 2009

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Company Code: BAZ**Active Code:** SFF**Use Site Category:** 13 and 14**EPA PC Code:** 118203

CITATION: Panek, M. 2006. Hydrolysis of ¹⁴C-BAS 800 H. Unpublished study performed, sponsored, and submitted by BASF Corporation, Research Triangle Park, North Carolina. BASF Reg. Doc. No.: 2005/7004259. BASF Study No.: 132680. Experiment started November 16, 2004 and completed January 30, 2006 (p. 12). Final report issued October 10, 2006. (MRID 47127823. PMRA Number: 1546926.)



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EPA DP Barcode: D349858
OECD Data Point:
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Chemical name:

IUPAC name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.

N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

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EXECUTIVE SUMMARY

The hydrolysis of [uracil-4-¹⁴C]- and [phenyl-U-¹⁴C]-labeled N'-{2-chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide (saflufenacil; BAS 800 H; radiochemical purities $\geq 98.9\%$), at 1.8-2.7 mg/L, was studied in the dark at $25 \pm 1^\circ\text{C}$ in sterile aqueous buffered pH 5 (0.01N acetate), pH 7 (0.01N TRIS) and pH 9 (0.01N TRIS) solutions for 30 days. The experiment was conducted in accordance with USEPA Pesticide Assessment Guidelines, Subdivision N, §161-1, and in compliance with USEPA FIFRA GLP standards (40 CFR 160). The test system consisted of glass vials (not further described) containing treated buffer solution (4 mL) that were capped and incubated in the dark; volatiles were not addressed. Vials of each pH/label solution were collected for analysis as follows:

pH 5 and 7/both labels: At 0, 1, 3, 8, 15, 21, and 30 days.

pH 9/uracil label: At 0, 0.75, 1, 1.75, 2, 3, 8, 15, 21, and 30 days.

pH 9/phenyl label: At 0, 0.12, 0.17, 0.25, 0.33, 1, 2, 3, 8, 15, 24, and 30 days.

Duplicate vials were collected at most sampling intervals; single samples were collected from the pH 9/uracil at 0.75, 1.75, and 2 days and the pH 9/phenyl at 0.12 and 0.25 days. Samples were directly analyzed by LSC and HPLC. [¹⁴C]Residues were identified by comparison to an unlabeled reference standard of saflufenacil (purity 99.9%) and four of its transformation products. Identifications were confirmed using LC/MS, LC-MS/MS, GC/MS and NMR.

During the study, the temperature of the buffer solutions was reported to be $25 \pm 1^\circ\text{C}$; no supporting data were provided. The pH of the buffer solutions ranged from 4.98-5.11 (pH 5), 6.97-7.12 (pH 7) and 8.56-9.04 (pH 9). The sterility was reported as having been verified by visual observation of the agar plates after incubation; no supporting data were provided.

In solutions treated with [uracil-4-¹⁴C]saflufenacil, overall [¹⁴C]residue recoveries averaged $102.1 \pm 1.2\%$ of the applied (range 100.0-104.7%) in the pH 5 buffer solution, $101.9 \pm 2.1\%$ of the applied (range 99.8-106.5%) in the pH 7 buffer solution and $97.7 \pm 1.5\%$ (range 94.8-100.1%) in the pH 9 buffer solution. In solutions treated with [phenyl-U-¹⁴C]saflufenacil, overall [¹⁴C]residue recoveries averaged $100.2 \pm 0.9\%$ of the applied (range 98.6-101.8%) in the pH 5 buffer solution, $100.4 \pm 1.1\%$ of the applied (range 98.3-102.1%) in the pH 7 buffer solution and $100.6 \pm 1.7\%$ (range 98.5-106.3%) in the pH 9 buffer solution. Recoveries in the pH 9/uracil solution were variable, but generally trended downward. There was no pattern of loss of material over time from the other buffer solutions.

Saflufenacil was stable in the pH 5 buffer solution. Based on first order linear regression analysis (Excel 2003), saflufenacil (combined labels) dissipated with half-lives of 248 days in the pH 7 buffer solution and 4.9 days in the pH 9 buffer solution. The half-life at pH 7 is of uncertain value because it is extrapolated well beyond the duration of the study. Four transformation products were identified:

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- M800H04 (chemical name not available; both labels);
- M800H07 (N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]-phenyl}-N'-methylurea; urea; in the phenyl label only);
- M800H15 (N-{4-chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]-phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide; ketohydrate; both labels); and
- M800H33 (1,1,1-trifluoroacetone; in the uracil label only).

All four compounds were major transformation products in the pH 9 buffer solutions, and were either minor or not detected in the pH 5 and pH 7 buffer solutions.

At **pH 5**, [^{14}C]saflufenacil (both labels) ranged from 99.5-102.8% of the applied throughout the study. No major transformation products were isolated. Minor transformation products M800H04 and M800H15 were each $\leq 0.7\%$ of the applied throughout the study, and unidentified [^{14}C]compounds were each $\leq 1\%$ of the applied.

At **pH 7**, [^{14}C]saflufenacil (both labels) decreased from an average of 100.2-100.3% of the applied at time 0 to 89.3-93.8% at 30 days posttreatment (study termination). No major transformation products were isolated. Minor transformation products were M800H07, M800H33, M800H04, and M800H15. M800H07 increased steadily to a maximum average of 8.6% of the applied (individual maximum of 9.2%) at 30 days posttreatment. M800H33 averaged a maximum of 4.5% of the applied, and M800H04 and M800H15 averaged maximums of 0.6% and 1.7-2.1%, respectively. Unidentified [^{14}C]compounds were each $\leq 1\%$ of the applied.

At **pH 9**, [^{14}C]saflufenacil (both labels) decreased from an average of 99.8-100.1% of the applied at time 0 to 51.9-57.5% at 2 days posttreatment, 14.4-25.0% at 8 days, and 1.1-3.1% at 30 days (study termination). In the **pH 9/uracil treatment**, three major transformation products (M800H33, M800H15, M800H04) were isolated and no minor transformation products were identified. M800H33 averaged a maximum of 72.2% of the applied (individual maximum of 74.0%) at 21 days posttreatment and was 71.7% at 30 days. M800H15 averaged a maximum of 21.8% of the applied (individual maximum of 22.1%) at 30 days posttreatment. M800H04 averaged a maximum of 12.4% of the applied (individual maximum of 12.9%) at 3 days posttreatment and was not detected at 21 and 30 days. Unidentified [^{14}C]compounds were each $\leq 4.9\%$ of the applied. In the **pH 9/phenyl treatment**, three major transformation products (M800H07, M800H15, M800H04) were isolated and no minor transformation products were identified. M800H07 and M800H15 averaged maximums of 76.7% and 21.3% of the applied (individual maximums of 76.9% and 21.5%), respectively, at 30 days posttreatment. M800H04 averaged a maximum of 9.7% of the applied (individual maximum of 9.9%) at 3 days posttreatment and was not detected at 30 days. Unidentified [^{14}C]compounds were each $\leq 2.1\%$ of the applied.

A transformation pathway for saflufenacil was provided by the study author. Saflufenacil degrades via the opening and cleavage of the uracil ring to M800H15 and M800H04, the latter of

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which further degrades to M800H07 and M800H33. Degradation is rapid under alkaline conditions and slow at neutral pHs; saflufenacil appears to be stable under acidic conditions.

RESULTS SYNOPSIS (Combined Labels):

pH	Half-life (days)	Transformation products	
		Major	Minor (identified)
5	Stable.	None.	N-{4-Chloro-2-fluoro-5- [({[isopropyl(methyl)amino]sulfonyl} amino)carbonyl]phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide (M800H15; ketohydrate) M800H04
7	248	None.	1,1,1-Trifluoroacetone (M800H33) N-{4-Chloro-2-fluoro-5- [({[isopropyl(methyl)amino]sulfonyl} amino)carbonyl]phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide (M800H15; ketohydrate) M800H04 N-{4-Chloro-2-fluoro-5- [({[isopropyl(methyl)amino]sulfonyl} amino)carbonyl]phenyl}-N'-methylurea (M800H07; urea).
9	4.93	1,1,1-Trifluoroacetone (M800H33) N-{4-Chloro-2-fluoro-5- [({[isopropyl(methyl)amino]sulfonyl} amino)carbonyl]phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide (M800H15; ketohydrate) M800H04 N-{4-Chloro-2-fluoro-5- [({[isopropyl(methyl)amino]sulfonyl} amino)carbonyl]phenyl}-N'-methylurea (M800H07; urea).	None.

Study Acceptability: This study is classified as **acceptable** to PMRA and USEPA and **reliable with restrictions** to DEWHA/APVMA (co-solvent concentration was not reported). No significant deviations from good scientific practices were noted.

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I. MATERIALS AND METHODS

GUIDELINE FOLLOWED: This study was conducted in accordance with USEPA Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-1 (1993; p. 12). Significant deviations from the objectives of Subdivision N guidelines include:

The co-solvent concentration was not reported. Co-solvent should not exceed 1% of test solutions.

Limits of detection and quantitation were not reported.

COMPLIANCE: This study was conducted in compliance with USEPA FIFRA GLP (40 CFR 160; pp. 3, 12). Signed and dated Data Confidentiality and Certification statements were provided (pp. 2, 5). Signed, but not dated GLP and Quality Assurance statements were provided (pp. 3-4).

A. MATERIALS:

1. Test Materials [Phenyl-U-¹⁴C] and [uracil-4-¹⁴C]saflufenacil (pp. 13-14).

Chemical Structure: See DER Attachment 1.

Description: Technical (pp. 13-14).

[Phenyl-U-¹⁴C]

Purity: Radiochemical purity: ≥98.9% (HPLC; pp. 13-14).
Batch No. 825-1085.
Analytical purity: 100.0% (p. 13).
Specific activity: 5.54 MBq/mg, 332400 dpm/μg.
Location of the radiolabel: Uniformly labeled on the phenyl ring (p. 6).

[Uracil-4-¹⁴C]

Purity: Radiochemical purity: ≥99% (HPLC; p. 14).
Batch No. 829-1017.
Analytical purity: 99.5% (p. 14).
Specific activity: 4.26 MBq/mg, 255600 dpm/μg.
Location of the radiolabel: At the 4-C position on the uracil ring (p. 6).

Storage conditions of test chemicals: The test material was stored frozen (0 to -30°C; p. 14). Reference substances were stored frozen, and the acids were stored at room temperature (p. 17). Reference substance solutions were stored frozen.

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Physico-chemical properties of saflufenacil:

Parameter		Value	Comment
Molecular weight (g/Mol)		500.86	
Molecular formula		C ₁₇ H ₁₇ ClF ₄ N ₄ O ₅ S	
Water solubility (mg/L)	pH 4, 20°C:	14 (pH 4, 20°C)	
	pH 5, 20°C:	25 (pH 5, 20°C)	
	pH 7, 20°C:	2100 (pH 7, 20°C)	
	pH 9, 20°C:	Not determined due to degradation.	
Vapor pressure	20°C:	4.5 x 10 ⁻¹⁵ Pa	Indicates nonvolatility.
	25°C:	2.0 x 10 ⁻¹⁴ Pa	
UV Absorption	pH 1, pH 7:	UV/VIS λ _{max} = 272 nm	Indicates possible susceptibility to direct photolysis at alkaline pH.
	pH 12:	UV/VIS λ _{max} = 309 nm	
pKa		4.41	Indicates neutrality at ambient pH.
K _{ow}		368	Indicates low potential to bioconcentrate.
log K _{ow}		2.56	
Stability of compound at room temperature		Stable for >2 yrs.	

Data obtained from Genari, 2007 (MRID 47127814); Beery, 2007 (MRID 47127815); Beery, 2006 (MRID 47127817); Vanhook, 2005 (MRID 47127818); Vanhook, 2005a (MRID 47127819); and Kroel, 2005 (MRID 47127821).

2. Buffer Solution: Buffer solutions were sterilized by autoclaving, except the pH 9 buffer solution that was used for a repeat of the phenyl label treatment, which was sterilized using a disposable filter unit (0.20 µm; p. 19). Buffer solutions were prepared with purified water (Burdick and Jackson High Purity Water) as follows:

Table 1: Description of buffer solutions.

pH	Type and molarity of buffer	Composition
5	0.01N Acetate	Sodium acetate trihydrate was dissolved in purified water and the pH adjusted to pH 5 using 1 M acetic acid.
7	0.01N TRIS	Trizma preset crystals were dissolved in purified water and the pH adjusted to pH 7 using 1 N sodium hydroxide.
9	0.01N TRIS	Trizma preset crystals were dissolved in purified water and the pH adjusted to pH 9 using 1 N sodium hydroxide.

Data obtained from p. 19 of the study report.

B. EXPERIMENTAL CONDITIONS

1. Preliminary Study: The hydrolysis of [uracil-4-¹⁴C]saflufenacil was studied for 8 days at 50 ± 2°C in sterile aqueous pH 5 (acetate), pH 7 (TRIS) and pH 9 (TRIS) buffer solutions at application solution concentrations of 2.92, 2.49, and 2.70 mg/L, respectively (pp. 19-20). The test solutions (4 mL) were pipetted into capped glass vials and placed in an incubator in the dark for 8 days. Single samples were collected at 0, 0.17, 1, 2, and 8 days posttreatment. The degradation rate of the samples was evaluated to determine appropriate sampling intervals. The

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study author reported that [uracil-4-¹⁴C]saflufenacil degraded rapidly in pH 9 buffer; therefore, additional early sampling intervals would be included in the definitive study. The actual rates of degradation were not determined by the study author, and concentrations of saflufenacil were not provided. No information regarding transformation products was provided.

2. Experimental conditions

Table 2: Experimental parameters

Parameters		Uracil label	Phenyl label
Duration of study		30 days.	
Test concentrations			
Nominal:		2.7 mg a.i./L.	pH 5: 2.2 mg a.i./L. pH 7: 2.2 mg a.i./L. pH 9: 1.75 mg a.i./L.
Measured ¹ :		pH 5: 2.73 -2.77 mg a.i./L. pH 7: 2.75 -2.77 mg a.i./L. pH 9: 2.75 -7.76 mg a.i./L.	pH 5: 2.21 mg a.i./L. pH 7: 2.15 -2.16 mg a.i./L. pH 9: 1.76- 1.77 mg a.i./L.
No. of replications		Duplicate samples were collected for each label at each interval; additional single samples were collected at pH 9 for establishment of the half-life.	
Preparation of test medium	Volume used/treatment	Bulk buffer solutions were treated with application solution and aliquots (4 mL) of treated buffer were transferred to individual vials.	
	Method of sterilization	All equipment and buffer solutions were sterilized by autoclaving; pH 9 buffer solutions were sterilized with a Nalgene filter unit (0.20 µm).	
	Co-solvent	Acetonitrile (concentration not reported).	
Test apparatus (type/material/volume)		Glass vials filled with "little headspace" with treated buffer solution (4 mL) were capped and incubated in the dark at 25 ± 1°C.	
Details of traps for volatile, if any		Volatile traps were not used.	
If no traps were used, is the test system closed/open?		The test vessels were closed using caps.	
Is there any indication of the test material adsorbing to the walls of the test apparatus?		None.	
Experimental conditions			
Temperature (°C):		25 ± 1°C.	
Lighting:		Dark.	
pH ranges:		pH 5: 4.98-5.04, pH 7: 6.97-7.04, pH 9: 8.97-9.04.	pH 5: 5.08-5.11, pH 7: 7.09-7.12, pH 9: 8.56-9.01.
Other details, if any		None.	

Data were obtained from pp. 18-20, 25, Tables 1-2, pp. 35-36 of the study report.

1 Bold values were set to 100% of the applied by the study author (p. 19).

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3. Supplementary Experiments: A supplementary experiment was performed to identify parent and transformation products using pH 10 buffer solutions incubated in the dark at 50°C (p. 20).

Four treatments were prepared as follows:

High Dose 1 and High Dose 2: mixtures of [¹⁴C]saflufenacil and unlabeled saflufenacil;

High Dose 3: 10 mg of [¹³C]saflufenacil and *ca.* 20 µg [¹⁴C]saflufenacil in 2 mL of ammonium deuterium oxide;

High Dose 4: 10 mg of [¹³C]saflufenacil and *ca.* 20 µg [¹⁴C]saflufenacil in 2 mL of ammonium hydroxide. The samples were analyzed using LC-MS, LC-MS/MS, GC/MS, and NMR (p. 27; Appendices 4-6, pp. 78-155).

4. Sampling:

Table 3: Sampling details.

Criteria	Uracil label	Phenyl label
Sampling intervals	pH 5: 0, 1, 3, 8, 15, 21, and 30 days. pH 7: 0, 1, 3, 8, 15, 21, and 30 days. pH 9: 0, 0.75, 1, 1.75, 2, 3, 8, 15, 21, and 30 days.	pH 5: 0, 1, 3, 8, 15, 21, and 30 days. pH 7: 0, 1, 3, 8, 15, 21, and 30 days. pH 9: 0, 0.12, 0.17, 0.25, 0.33, 1, 2, 3, 8, 15, 24, and 30 days.
Sampling method	Duplicate samples of each label were collected at each interval, except, single samples were collected from pH 9 at 0.75, 1.75, and 2 days for the uracil label and at 0.12 and 0.25 days for the phenyl label.	
Method of collection of CO ₂ and organic volatile compounds	Volatiles were not collected.	
Sampling intervals/times for: pH measurement:	At each sampling interval.	At each sampling interval.
Sterility check:	None.	At 15 and 30 days (pH 5 and 7) and at 8 and 24 days (pH 9).
Sample storage before analysis	All samples were stored in the freezer. Samples in pH 9 buffer solution were analyzed within 12 hours, and samples in pH 5 and 7 were analyzed within 24 hours.	
Other observation, if any:	None.	

Data were obtained from pp. 20-21, 24-25, Table 1, p. 35, and Appendix 1, Table A1.1-A1.2, pp. 74-75 of the study report.

C. ANALYTICAL METHODS

Extraction/clean up/concentration methods: Samples were analyzed as collected, without manipulation or modification (p. 21).

Volatile residue determination: Volatiles were not trapped.

Total ¹⁴C measurement: Three replicates of each sample were analyzed for total [¹⁴C]residues using LSC (p. 21).

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Derivatization method, if used: A solution of 2,4-dinitrophenylhydrazine (DNP) was prepared by dissolving DNP (1 g) in concentrated sulfuric acid (5 mL) and adding it to a mixture of water:denatured ethanol (7 mL:25 mL; p. 23). The DNP reagent (2 mL) was reacted with trifluoroacetone (20 µL) in denatured ethanol (2 mL). The solution was centrifuged, the solution decanted, and the crystals dissolved in ethanol (*ca.* 300 µL) to produce DNP hydrazone of trifluoroacetone.

Identification and quantification of parent compound: An aliquot (0.050 mL) of each test sample was analyzed directly by HPLC with two systems (BASF No. 1581 and 1260) under the following conditions: Waters YMC ODC-AQ (250 mm x 4.6 mm, 5 µm) column, gradient mobile phase for methods BAS800 to BAS8006 consisting of (A) 0.5% formic acid in water and (B) acetonitrile and for method BAS8007 consisting of (A) water and (B) acetonitrile, flow rate 1 mL/min, with radio and UV (280 nm) detection (pp. 21-23).

Gradient conditions for the different methods employed are as follows:

BAS800/BAS8001/BAS8002		(BAS8004/BAS8007)/BAS8005/BAS8006	
Time (min)	% A:% B	Time (min)	% A:% B
0.00	90:10	0.00	90:10
1.00/1.00/6.00	90:10	6.00/6.00/10.00	90:10
15.00/15.00/20.00	10:90	36.00	10:90
18.00/21.00/26.00	10:90	38.00	10:90
20.00/23.00/28.00	90:10	38.50	90:10
22.00/25.00/30.00	90:10	40.00	90:10

The HPLC results were confirmed with the supplementary experiment solutions using two LC/MS methods, in both negative and positive ion mode. The first used atmospheric pressure chemical ionization under the following conditions: Phenomenex Columbus (100 x 2.0 mm, 5 µm) column, gradient mobile phase consisting of (A) 98% water, 2% methanol, 0.1% formic acid, and 4 mM ammonium formate and (B) 98% methanol, 2% water, 0.1% formic acid, and 4 mM ammonium formate [percent A:B, v:v; 0.1 min, 98:2; 10.0 min, 2:98; 20.0 min, 2:98; 20.1 min, 98:2; 25.0 min, 98:2], flow rate 0.40 mL/min, with radio detection (Appendix 4, p. 81).

The second used electrospray ionization under the following conditions: Phenomenex Columbus (50 x 2.0 mm, 5 µm) column, gradient mobile phase consisting of (A) water, 0.1% formic acid, and 4 mM ammonium formate and (B) methanol, 0.1% formic acid, and 4 mM ammonium formate [percent A:B, v:v; 0.1 min, 95:5; 2.0 min, 5:95; 10.0 min, 5:95; 10.5 min, 95:5; 13.0 min, 95:5], flow rate 0.30 mL/min, with radio detection (Appendix 4, pp. 81-82).

Samples were cochromatographed with an unlabeled reference standard of saflufenacil (Appendix 4, p. 82).

Identification and quantification of transformation products: Transformation products were quantified using HPLC, and were confirmed using the supplementary experiment solutions with LC-MS, LC-MS/MS, GC/MS (used to identify the volatile transformation product) and NMR (p.

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23; Appendix 4, p. 81; Appendix 5, pp. 120-154). Samples were cochromatographed with unlabeled reference standards of:

Compound name	IUPAC name	Reference standard No.	Purity
BAS 800 H (Saflufenacil)	N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.	4054449	99.9%
BAS 800 H ([uracil-5- ¹³ C and benzamide-carbonyl- ¹³ C]saflufenacil)	N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.	4054449	99.87%
M800H07	N-{4-chloro-2-fluoro-5-[[([isopropyl(methyl)amino]-sulfonyl)amino]carbonyl]-phenyl}-N'-methylurea	4775453	95.4%
None	3,3,3-Trifluoropropionic acid.	--	99.9%
None	4,4,4-Trifluorobutyric acid.	--	98.8%
M800H33	1,1,1-Trifluoroacetone.	--	99.0%

Data obtained from pp. 15-17 of the study report.

Detection limits (LOD, LOQ) for the parent compound: The Limits of Quantitation and Detection were not reported.

Detection limits (LOD, LOQ) for the transformation products: The Limits of Quantitation and Detection were not reported.

II. RESULTS AND DISCUSSION

A. TEST CONDITIONS: During the study, the temperature of the buffer solutions was reported to be maintained at $25 \pm 1^\circ\text{C}$; no supporting data were provided. The pH of the buffer solutions ranged from 4.98-5.11 (pH 5), 6.97-7.12 (pH 7) and 8.56-9.04 (pH 9; Table 1, p. 35). The sterility was reported as verified by "visual observation of the agar plates after incubation;" no supporting data were provided (pp. 6, 25).

B. MASS BALANCE: In the uracil label, overall recoveries of [¹⁴C]residues averaged $102.1 \pm 1.2\%$ of the applied (range 100.0-104.7%) from the pH 5 buffer solution, $101.9 \pm 2.1\%$ of the applied (range 99.8-106.5%) from the pH 7 buffer solution and $97.7 \pm 1.5\%$ (range 94.8-100.1%) from the pH 9 buffer solution (Table 3, p. 37; DER Attachment 2).

In the phenyl label, overall recoveries of [¹⁴C]residues averaged $100.2 \pm 0.9\%$ of the applied (range 98.6-101.8%) from the pH 5 buffer solution, $100.4 \pm 1.1\%$ of the applied (range 98.3-102.1%) from the pH 7 buffer solution and $100.6 \pm 1.7\%$ (range 98.5-106.3%) from the pH 9 buffer solution (Table 3, p. 37; DER Attachment 2).

Recoveries in the uracil label at pH 9 were variable, but generally trended downward. There was no pattern of loss of material over time from the other buffer solutions.

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Table 4a: Hydrolysis of [uracil-4-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 5 and 25°C.

Compound t_R ~minute ¹	Sampling times (days)						
	0	1	3	8	15	21	30
Saflufenacil (BAS 800 H) ~19.0 (~31.0)	100.8 \pm 1.1	101.1 \pm 1.2	102.2 \pm 0.6	102.8 \pm 0.6	101.4 \pm 0.8	101.7 \pm 0.1	101.1 \pm 0.6
Trifluoroacetone ~5.1 (~8.3)	--	--	--	--	--	--	--
Unk 16.2 ~16.2	--	--	--	0.6 \pm 0.2	0.3 \pm 0.2	0.9, ND	0.3 \pm 0.2
M800H15 ~17.6 (~27.8)	--	--	--	--	--	--	ND, 0.2
M800H04 ~18.3 (~28.6)	--	--	--	ND, 0.7	ND, 0.6	--	0.4 \pm 0.2
Unk 18.5-18.6 ~18.5	--	--	--	--	--	--	0.2, ND
Unk 20.8 ~20.8	--	--	--	ND, 0.4	ND, 0.4	--	0.3, ND
Other ²	--	--	--	--	--	0.2, ND	0.2, ND
CO ₂	Volatiles were not collected.						
Volatile organics	Volatiles were not collected.						
Total Recovery	100.8 \pm 1.1	101.1 \pm 1.2	102.2 \pm 0.6	103.9 \pm 1.2	102.2 \pm 0.3	102.5 \pm 0.4	102.2 \pm 1.3

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 10, p. 44 of the study report and DER Attachment 2. The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 Retention times are for HPLC method BAS8002, retention times in parentheses are for HPLC method BAS8004.

2 Sum of small peaks found that did not correspond to other time intervals.

ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

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Table 4b: Hydrolysis of [phenyl-U-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 5 and 25°C.

Compound t_R ~minute ¹	Sampling times (days)						
	0	1	3	8	15	21	30
Saflufenacil (BAS 800 H) ~30.7 (~19.0)	100.1 \pm 0.1	99.5 \pm 1.3	99.7 \pm 0.1	100.4 \pm 0.7	99.6 \pm 0.9	100.4 \pm 2.0	100.8 \pm 0.9
Unk 24.0 ~24.0	--	--	--	--	0.7 \pm 0.2	--	--
M800H07 ~25.7	--	--	--	--	--	--	--
Unk 26.8 ~26.8	--	--	--	--	0.4, ND	--	--
M800H15 ~27.6 (~17.6)	--	--	--	--	0.2, ND	--	--
CO ₂	Volatiles were not collected.						
Volatile organics	Volatiles were not collected.						
Total Recovery	100.1 \pm 0.1	99.5 \pm 1.3	99.7 \pm 0.1	100.4 \pm 0.7	100.5 \pm 0.4	100.4 \pm 2.0	100.8 \pm 0.9

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 5, p. 39 of the study report and DER Attachment 2. The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 Retention times are for HPLC method BAS8004, retention times in parentheses are for HPLC method BAS8002. ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

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Table 4c: Hydrolysis of [uracil-4-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean \pm s.d., n = 2), at pH 7 and 25°C.

Compound t_R ~minute ¹	Sampling times (days)						
	0	1	3	8	15	21	30
Saflufenacil (BAS 800 H) ~19.0 (~31.0)	100.3 \pm 0.4	100.5 \pm 1.0	101.4 \pm 1.4	99.1 \pm 0.8	99.7 \pm 3.0	98.8 \pm 4.1	93.8 \pm 3.3
Trifluoroacetone ~5.1 (~8.3)	--	--	--	1.4 \pm 0.6	2.4 \pm 0.1	4.1 \pm 0.6	4.5 \pm 0.3
Unk 16.2 ~16.2	--	--	--	0.8 \pm 0.1	0.4 \pm 0.0	ND, 0.71	0.8, ND
M800H15 ~17.6 (~27.8)	--	--	--	0.5, ND	0.7 \pm 0.1	0.8 \pm 0.1	1.7 \pm 0.2
M800H04 ~18.3 (~28.6)	--	--	--	0.2, ND	0.6 \pm 0.4	0.2 \pm 0.0	1.0, ND
Unk 20.8 ~20.8	--	--	--	0.2 \pm 0.0	--	--	0.1, ND
CO ₂	Volatiles were not collected.						
Volatile organics	Volatiles were not collected.						
Total Recovery	100.3 \pm 0.4	100.5 \pm 1.0	101.4 \pm 1.4	101.9 \pm 0.9	103.8 \pm 3.5	104.4 \pm 3.0	101.0 \pm 1.5

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 12, p. 46 of the study report and DER Attachment 2. The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 Retention times are for HPLC method BAS8002, retention times in parentheses are for HPLC method BAS8004. ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

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Table 4d: Hydrolysis of [phenyl-U-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean ± s.d., n = 2), at pH 7 and 25°C.

Compound t _R ~minute ¹	Sampling times (days)						
	0	1	3	8	15	21	30
Saflufenacil (BAS 800 H) ~30.7 (~19.0)	100.2 ± 0.3	99.3 ± 1.1	99.2 ± 1.3	99.6 ± 0.6	94.8 ± 0.8	94.4 ± 0.7	89.3 ± 0.8
Unk 24.0 ~24.0	--	--	--	--	0.7, ND	--	--
M800H07 ~25.7	--	--	--	1.8 ± 0.2	3.8 ± 0.5	5.3 ± 0.6	8.6 ± 0.8
M800H15 ~27.6 (~17.6)	--	--	--	0.2 ± 0.0	1.2 ± 0.3	1.5 ± 0.2	2.1 ± 0.4
M800H04 ~28.5 (~18.3)	--	--	--	0.3 ± 0.1	0.6 ± 0.1	--	0.7, ND
Unk 39.3 ~39.3	--	0.9, ND	--	--	--	--	--
CO ₂	Volatiles were not collected.						
Volatile organics	Volatiles were not collected.						
Total Recovery	100.2 ± 0.3	99.7 ± 0.4	99.2 ± 1.3	101.9 ± 0.4	100.6 ± 2.1	101.2 ± 0.3	100.3 ± 0.3

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 6, p. 40 of the study report and DER Attachment 2. The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 Retention times are for HPLC method BAS8004, retention times in parentheses are for HPLC method BAS8002. ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

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Table 4e: Hydrolysis of [uracil-4-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean \pm s.d., when n = 2), at pH 9 and 25°C.

Compound t_R ~minute ²	Sampling times (days)									
	0	0.75 ¹	1	1.75 ¹	2 ¹	3	8	15	21	30
Saflufenacil (BAS 800 H) ~19.0 (~31.0)	100.1 \pm 0.1	77.7	72.3 \pm 0.8	55.4	51.9	41.4 \pm 0.7	14.4 \pm 0.7	3.8 \pm 0.3	1.3 \pm 0.2	1.1 \pm 0.5
Trifluoroacetone ~5.1 (~8.3)	--	8.2	10.7 \pm 0.1	21.9	25.8	32.4 \pm 2.5	56.8 \pm 0.4	68.7 \pm 0.7	72.2 \pm 2.5	71.7 \pm 2.1
Unk 6.4 ~6.4	--	--	--	--	--	ND, 4.9	--	--	--	--
M800H15 ~17.6 (~27.8)	--	1.8	2.6 \pm 0.2	4.5	4.5	6.2 \pm 0.5	14.0 \pm 0.5	19.3 \pm 0.3	21.7 \pm 0.0	21.8 \pm 0.3
M800H04 ~18.3 (~28.6)	--	8.2	7.8 \pm 0.9	11.2	12.2	12.4 \pm 0.7	7.9 \pm 0.1	2.1 \pm 0.1	--	--
Unk 18.5-18.6 ~18.6	--	2.0	2.8 \pm 0.3	1.5	1.4	1.4 \pm 0.6	0.9 \pm 0.1	--	--	--
Unk 20.1 ~20.1	--	1.6	0.9 \pm 0.2	4.0	2.2	2.5 \pm 0.4	2.6 \pm 0.3	1.6 \pm 0.3	0.6 \pm 0.4	0.4, ND
CO ₂	Volatiles were not collected.									
Volatile organics	Volatiles were not collected.									
Total Recovery	100.1 \pm 0.1	99.5	96.9 \pm 0.1	98.4	97.9	98.7 \pm 1.9	96.7 \pm 0.2	96.8 \pm 0.1	96.6 \pm 2.5	96.6 \pm 1.1

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 14, p. 48 of the study report and DER Attachment 2.
The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 A single sample was collected at this interval.

2 Retention times are for HPLC method BAS8002, retention times in parentheses are for HPLC method BAS8004.

ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

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Table 4f: Hydrolysis of [phenyl-U-¹⁴C]saflufenacil, expressed as percentage of the applied radioactivity (mean ± s.d., when n = 2), at pH 9 and 25°C.

Compound t _R ~minute ²	Sampling times (days)											
	0	0.12 ¹	0.17	0.25 ¹	0.33	1	2	3	8	15	24	30
Saflufenacil (BAS 800 H) ~31.0 (~19.0)	99.8 ± 0.3	100.1	95.8 ± 1.7	94.0	89.1 ± 0.9	74.6 ± 4.3	57.5 ± 4.1	48.2 ± 1.0	25.0 ± 5.8	12.0 ± 9.7	11.1 ± 1.9	3.1 ± 3.6
M800H07 ~25.6	--	--	0.9 ± 0.2	1.6	2.4 ± 0.2	12.3 ± 0.8	23.8 ± 1.3	32.5 ± 0.5	53.5 ± 4.6	66.5 ± 4.5	70.0 ± 2.0	76.7 ± 0.4
M800H15 ~27.8 (~17.6)	--	--	--, 0.84	1.1	2.1 ± 0.1	3.8 ± 0.3	7.6 ± 1.7	9.0 ± 0.1	15.8 ± 0.8	18.3 ± 2.8	20.1 ± 0.2	21.3 ± 0.3
M800H04 ~28.6 (~18.3)	--	--	1.4 ± 0.0	2.3	2.8 ± 0.8	6.5 ± 0.1	8.8 ± 1.8	9.7 ± 0.4	5.9 ± 0.5	3.1 ± 0.7	1.7 ± 0.3	ND
Unk 29.3 ~29.3	--	--	--, 0.6	1.5	0.8 ± 0.2	0.9 ± 0.3	0.6 ± 0.2	--	--	--	--	--
Unk 29.8 ~29.8	--	--	1.5 ± 0.4	--	2.1 ± 0.3	1.9 ± 0.8	1.7 ± 0.7	ND, 0.5	--	--	--	--
Other ³	--	--	--	--	0.5 ± 0.0	--, 1.03	--	--	--	0.7, --	1.0 ± 0.2	1.1 ± 0.3
CO ₂	Volatiles were not collected.											
Volatile organics	Volatiles were not collected.											
Total Recovery	99.8 ± 0.4	100.1	100.4 ± 0.9	100.4	99.8 ± 0.2	100.5 ± 1.2	100.0 ± 0.0	99.6 ± 0.6	100.2 ± 0.2	100.3 ± 2.5	103.8 ± 3.6	102.2 ± 3.2

Means and standard deviations calculated by the reviewer using data obtained from Table 3, p. 37 and Table 8, p. 42 of the study report and DER Attachment 2. The study author presented data to both one and two decimal places; values rounded to one decimal place by reviewer.

1 A single sample was collected at this interval.

1 Retention times are for HPLC method BAS8004, retention times in parentheses are for HPLC method BAS8002. 3 Sum of small peaks found that did not correspond to other time intervals.

ND = Not Detected.

-- Blank cells in the original data tables. Although these are most likely "Not Detected", "ND" is used in the tables when a detection occurred in one of the two replicate samples.

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C. TRANSFORMATION OF PARENT COMPOUND: At pH 5, [uracil-4-¹⁴C]saflufenacil ranged from 100.8-102.8% of the applied throughout the study (Table 10, p. 44; DER Attachment 2). At pH 7, [¹⁴C]saflufenacil decreased from an average of 100.3% of the applied at time 0 to 93.8% at 30 days posttreatment (study termination, Table 12, p. 46). At pH 9, [¹⁴C]saflufenacil decreased from an average of 100.1% of the applied at time 0 to 51.86% at 2 days to 14.4% at 8 days, and was 1.1% at 30 days posttreatment (study termination, Table 14, p. 48).

At pH 5, [phenyl-U-¹⁴C]saflufenacil ranged from 99.5-100.8% of the applied throughout the study (Table 5, p. 39; DER Attachment 2). At pH 7, [¹⁴C]saflufenacil decreased from an average of 100.2% of the applied at time 0 to 89.3% at 30 days posttreatment (study termination, Table 6, p. 40). At pH 9, [¹⁴C]saflufenacil decreased from an average of 99.8% of the applied at time 0 to 48.2% at 3 days to 25.0% at 8 days, and was 3.1% at 30 days posttreatment (study termination, Table 8, p. 42).

HALF-LIVES/DT50/DT90: Based on first order linear regression analysis (Excel 2003), [uracil-4-¹⁴C]saflufenacil dissipated from the pH 7 and 9 buffer solutions with reviewer-calculated half-lives of 347 and 4.22 days, respectively (Table 12, p. 46, Table 14, p. 48, DER Attachment 2). [Uracil-4-¹⁴C]saflufenacil was stable in the pH 5 buffer solution. The half-life value for the pH 7 buffer solution is of highly uncertain value since it is extrapolated well beyond the duration of the study.

Based on first order linear regression analysis (Excel 2003), [phenyl-U-¹⁴C]saflufenacil dissipated from the pH 7 and 9 buffer solutions with reviewer-calculated half-lives of 193 and 5.87 days, respectively (Table 6, p. 40, Table 8, p. 42, DER Attachment 2). [Phenyl-U-¹⁴C]saflufenacil was stable in the pH 5 buffer solution. The half-life value for the pH 7 buffer solution is of highly uncertain value since it is extrapolated well beyond the duration of the study.

In the combined labels, saflufenacil dissipated from the pH 7 and 9 buffer solutions with reviewer-calculated half-lives of 248 days and 4.93 days, respectively.

The study author's calculated DT50 values for [uracil-4-¹⁴C]-labeled and [phenyl-U-¹⁴C]-labeled saflufenacil, using first order kinetics, were consistent with reviewer-calculated values (pp. 24, 32; Tables 16-17, pp. 50-51).

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Half-lives/DT50/DT90

pH	First order linear			Observed DT50 (days)	Observed DT90 (days)
	Half-life (days) ¹	Regression equation	r ²		
Uracil label					
5	Stable.			---	---
7	347	y = -0.002x + 4.6174	0.4904	---	---
9	4.22	y = -0.1643x + 4.263	0.9457	2-3	8-15
Phenyl label					
5	Stable.			---	---
7	193	y = -0.0036x + 4.6108	0.9056	---	---
9	5.87	y = -0.118x + 4.4345	0.8431	2-3	24-30
Combined labels					
5	Stable.			---	---
7	248	y = -0.0028x + 4.6141	0.6189	---	---
9	4.93	y = -0.1407x + 4.3599	0.8533	---	---

¹ Calculated by the reviewer using data obtained from Table 6, p. 40, Table 8, p. 42, Table 12, p. 46, and Table 14, p. 48 of the study report (DER Attachment 2).

--- = No observation.

TRANSFORMATION PRODUCTS: Four major transformation products were identified in pH 9 buffer solutions; these same products were the minor transformation products isolated in the pH 5 and 7 buffer solutions:

- M800H33 (1,1,1-Trifluoroacetone),
- M800H15 (N-{4-Chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide),
- M800H04, and
- M800H07 (N-{4-Chloro-2-fluoro-5-[(isopropyl(methyl)amino)sulfonyl]amino}carbonyl]phenyl}-N'-methylurea).

At pH 5, M800H15 was a maximum of 0.2% (single replicate) of the applied in the uracil and phenyl label, respectively (Table 5, p. 39; Table 10, p. 44; DER Attachment 2). M800H04 was a maximum of 0.7% in the uracil label. In the uracil label, unknowns and other unidentified radioactivity each totaled less than 1% of the applied. In the phenyl label, unknowns each totaled less than 1% of the applied.

At pH 7 in the uracil label, M800H33, M800H15, and M800H04 were maximum averages of 4.5%, 1.7%, and 0.6% of the applied, respectively (Table 12, p. 46; DER Attachment 2). Unknowns each totaled less than 1% of the applied. In the phenyl label, M800H07, M800H15, and M800H04 were maximum averages of 8.6%, 2.1%, and 0.6% of the applied, respectively (Table 6, p. 40). Unknowns each totaled less than 1% of the applied.

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At pH 9 in the uracil label, M800H15 was a maximum average of 21.8% of the applied (individual maximum of 22.1%) at 30 days posttreatment (study termination; Table 14, p. 48; DER Attachment 2). M800H04 was a maximum average of 12.4% of the applied (individual maximum of 12.9%) at 3 days, and was not reported as present at study termination. M800H33 was a maximum average of 72.2% (individual maximum of 74.0%) at 21 days, and was 71.7% at study termination. Unknowns were each $\leq 4.9\%$ of the applied.

At pH 9 in the phenyl label, M800H15 was a maximum average of 21.3% of the applied (individual maximum of 21.5%) at 30 days posttreatment (study termination; Table 8, p. 42; DER Attachment 2). M800H07 was a maximum average of 76.7% (individual maximum of 76.9%) at 30 days posttreatment (study termination). M800H04 was a maximum average of 9.7% (individual maximum of 9.9%) at 3 days, and was not detected at study termination. Unknowns and other unidentified radioactivity were each $\leq 2.1\%$ of the applied.

For the combined labels at pH 9, M800H04 degraded from peak concentrations at 3 days posttreatment to final detections at 24 days posttreatment, with a half-life of 7.04 days.

Table 5: Chemical names and CAS numbers for the transformation products of saflufenacil.

Applicants Code Name	CAS Number	Chemical Name	Chemical Formula	MW (g/mol)	Smiles String
M800H04	---	---	$C_{17}H_{19}ClF_4N_4O_6S$	518	---
M800H15 ¹ (Ketohydrate)	---	N-{4-Chloro-2-fluoro-5-[[{isopropyl(methyl)amino}sulfonyl]amino]carbonyl]phenyl}-4-4-4-trifluoro-3,3-dihydroxybutanamide	---	479	---
M800H07 ¹ (Urea)	---	N-{4-Chloro-2-fluoro-5-[[{isopropyl(methyl)amino}sulfonyl]amino]carbonyl]phenyl}-N'-methylurea	$C_3H_{18}ClFN_4O_4S$	380	---
M800H33	421-50-1	1,1,1-Trifluoroacetone	$C_3H_3F_3O$	112	---

Data obtained from pp. 16-17, 28-29; Figure 1, p. 53 of study report.

1 Names generated by ISIS draw.

--- = Not reported.

VOLATILIZATION: Volatiles were not collected.

TRANSFORMATION PATHWAY: A transformation pathway for saflufenacil was provided by the study author (p. 32; Figure 6, p. 58). Saflufenacil degrades in basic aqueous conditions through the opening and cleavage of the uracil ring to M800H15 and M800H04, the latter of which further degrades to M800H07 and M800H33. At a neutral pH, degradation is slow but follows the same pathway; M800H07 is the only transformation product approaching 10% of the applied.

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D. SUPPLEMENTARY EXPERIMENT-RESULTS: Results of high concentration supplementary experiments conducted at 50°C were incorporated into the main study results.

III. STUDY DEFICIENCIES

1. The co-solvent concentration was not reported. Co-solvent should not exceed 1% of test solutions.
2. Limits of detection and quantitation were not reported. This does not affect the acceptability of the study.

IV. REVIEWER'S COMMENTS

1. The pH 7 and 9 buffer solutions were prepared using TRIS. The study author did not demonstrate that the TRIS did not interact with the test substance or its transformation products.
2. The study author reported that the sterility of the test solutions was verified by "visual observation of the agar plates after incubation," but no supporting data were provided. No data were provided to verify that the temperature was held at $25 \pm 1^\circ\text{C}$ (p. 19).
3. The chemical name for M800H04 was not provided. A structure was provided.
4. The application rate was selected to be high enough for analysis, but within the water solubility of the test substance (p. 19).

V. REFERENCES

1. U.S. Environmental Protection Agency. 1982. Pesticide Assessment Guidelines, Subdivision N, Chemistry: Environmental Fate, Section 161-1. Hydrolysis studies. Office of Pesticide and Toxic Substances, Washington, DC. EPA 540/9-82-021.
2. U.S. Environmental Protection Agency. 1989. FIFRA Accelerated Reregistration, Phase 3 Technical Guidance. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 540/09-90-078.
3. U.S. Environmental Protection Agency. 1993. Pesticide Registration Rejection Rate Analysis - Environmental Fate. Office of the Prevention, Pesticides, and Toxic Substances, Washington, DC. EPA 738-R-93-010.

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

4. Ta, C., and J. Trollinger. 2007. Aqueous photolysis of 14C-BAS 800 H. Unpublished study performed, sponsored, and submitted by BASF Corporation, Research Triangle Park, North Carolina. BASF Study Protocol ID No.: 132683. BASF Doc. ID No.: 2007/7009413.

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Attachment 1: Structure of Parent Compound and Transformation Products

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

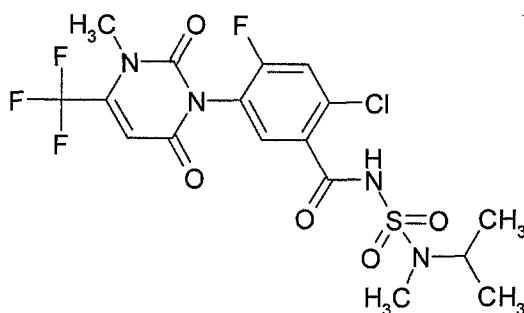
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

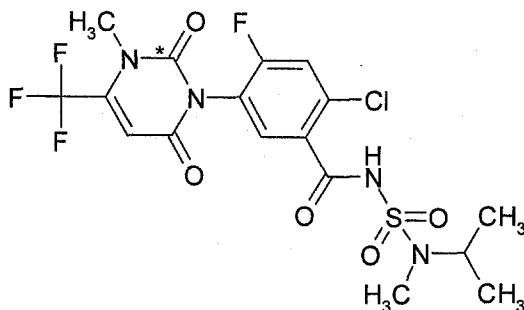
SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

Unlabeled



[Uracil-4-¹⁴C]Saflufenacil



* = Location of the radiolabel.

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926
PMRA Submission Number 2008-0431

EPA MRID Number 47127823

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

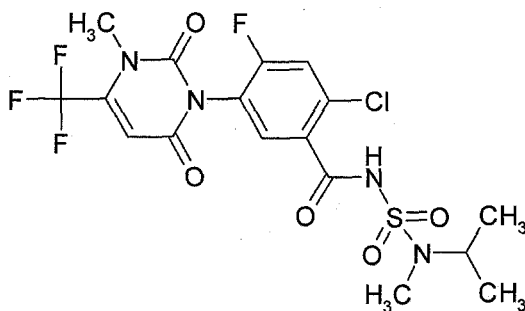
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

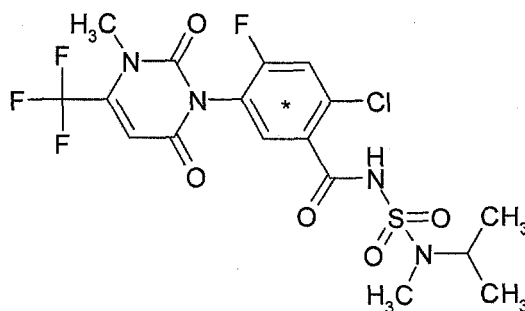
SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

Unlabeled



[Phenyl-U-¹⁴C]Saflufenacil



* = Location of the radiolabel.

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Identified Compounds

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

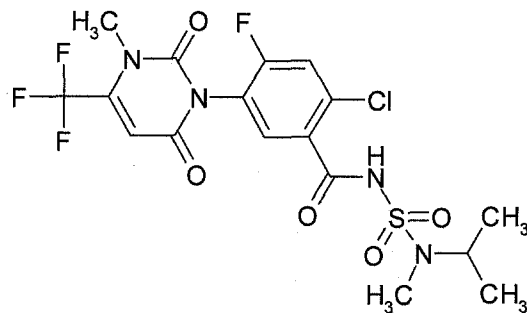
IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

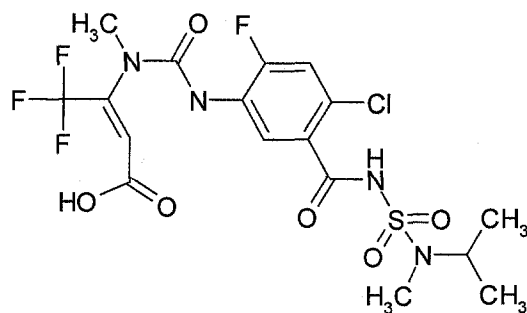


M800H04

IUPAC Name: Not reported.

CAS Name: Not reported.

CAS Number: Not reported.



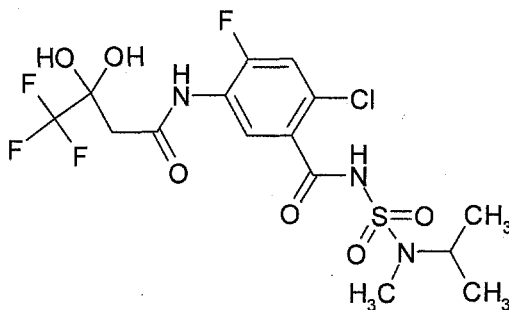
Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926
PMRA Submission Number 2008-0431

EPA MRID Number 47127823

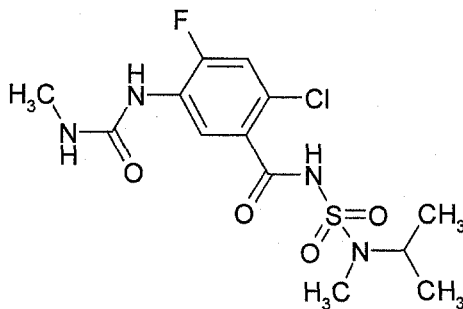
M800H15 [M800H15-ketohydrate, "Ketohydrate", 5264357]

IUPAC Name: N-{4-Chloro-2-fluoro-5-
[([isopropyl(methyl)amino]sulfonyl)amino)carbonyl]phenyl}-4-4-4-
trifluoro-3,3-dihydroxybutanamide.
CAS Name: Not reported.
CAS Number: Not reported.



M800H07 [4775453]

IUPAC Name: N-{4-Chloro-2-fluoro-5-
[([isopropyl(methyl)amino]sulfonyl)amino)carbonyl]phenyl}-N'-
methylurea.
CAS Name: Not reported.
CAS Number: Not reported.



Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

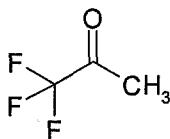
PMRA Submission Number 2008-0431

1,1,1-Trifluoroacetone [M800H33, TF acetone]

IUPAC Name: 1,1,1-Trifluoroacetone.

CAS Name: Not reported.

CAS Number: 421-50-1.



Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926

EPA MRID Number 47127823

PMRA Submission Number 2008-0431

Unidentified Reference Compounds

Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926
PMRA Submission Number 2008-0431

EPA MRID Number 47127823

Saflufenacil [BAS 800 H, CL No. 433379, 4054449, AC 433,379]

IUPAC Name: N'-{2-Chloro-4-fluoro-5-[1,2,3,6-tetrahydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)pyrimidin-1-yl]benzoyl}-N-isopropyl-N-methylsulfamide.
N'-[2-Chloro-4-fluoro-5-(3-methyl-2,6-dioxo-4-(trifluoromethyl)-3,6-dihydro-1(2H)-pyrimidinyl)benzoyl]-N-isopropyl-N-methylsulfamide.

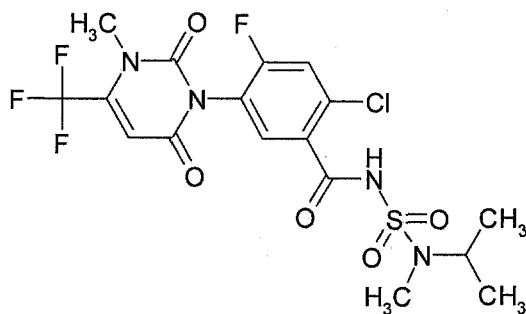
CAS Name: 2-Chloro-5-[3,6-dihydro-3-methyl-2,6-dioxo-4-(trifluoromethyl)-1(2H)-pyrimidinyl]-4-fluoro-N-[[methyl(1-methylethyl)amino]sulfonyl]benzamide.

CAS Number: 372137-35-4.

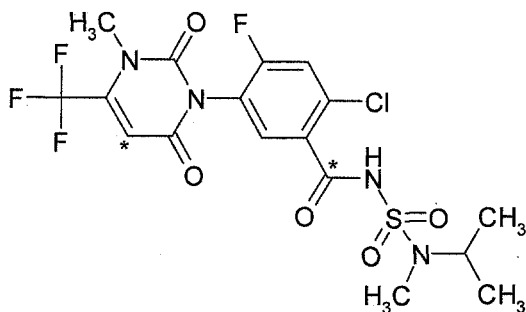
SMILES String: N1(C)C(C(F)(F)F)=CC(=O)N(C2=CC(C(=O)NS(=O)(=O)N(C)C(C)C)=C(Cl)C=C2F)C1=O (EPI Suite v3.12 SMILES string from ISIS .MOL).

Empirical formula: C₁₇H₁₇ClF₄N₄O₅S **Molecular formula:** C₁₇H₁₇ClF₄N₄O₅S

Unlabeled



[Uracil-5-¹³C] and [Benzamide-carbonyl-¹³C] Saflufenacil



* = Location of the radiolabel.

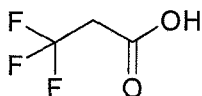
Data Evaluation Record on the hydrolysis of saflufenacil (BAS 800 H)

PMRA Document Number 1546926
PMRA Submission Number 2008-0431

EPA MRID Number 47127823

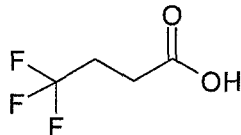
3,3,3-Trifluoropropionic acid

IUPAC Name: 3,3,3-Trifluoropropionic acid.
CAS Name: Not reported.
CAS Number: 2516-99-6.



4,4,4-Trifluorobutyric acid

IUPAC Name: 4,4,4-Trifluorobutyric acid.
CAS Name: Not reported.
CAS Number: 406-93-9.



Attachment 2: Excel Spreadsheets

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

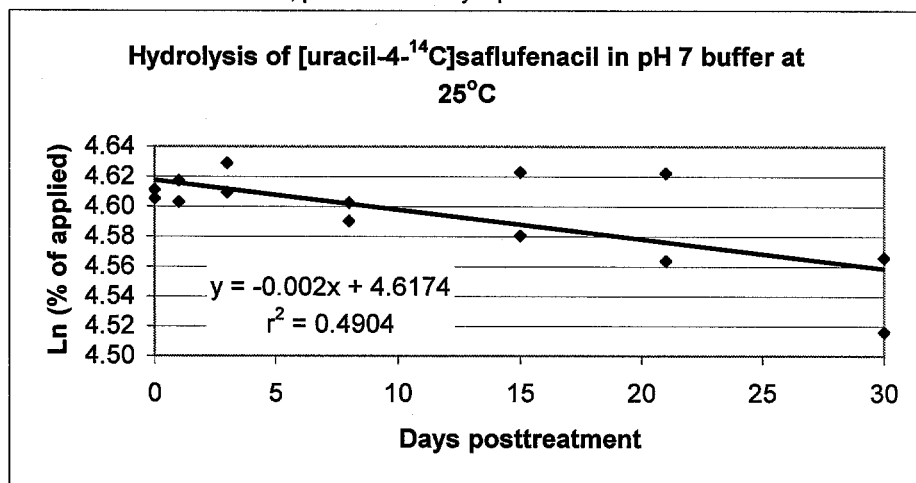
Uracil Label at pH 7

Half-life:

346.57 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.00	4.6052
0	100.58	4.6110
1	99.77	4.6029
1	101.19	4.6170
3	102.40	4.6289
3	100.42	4.6094
8	98.52	4.5903
8	99.72	4.6024
15	101.77	4.6227
15	97.57	4.5806
21	101.71	4.6221
21	95.92	4.5635
30	91.46	4.5159
30	96.13	4.5657

Data obtained from Table 12, p. 46 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.70031682
R Square	0.49044364
Adjusted R Square	0.44798061
Standard Error	0.02271369
Observations	14

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	0.005958729	0.005959	11.5499	0.005284201
Residual	12	0.006190942	0.000516		
Total	13	0.012149671			

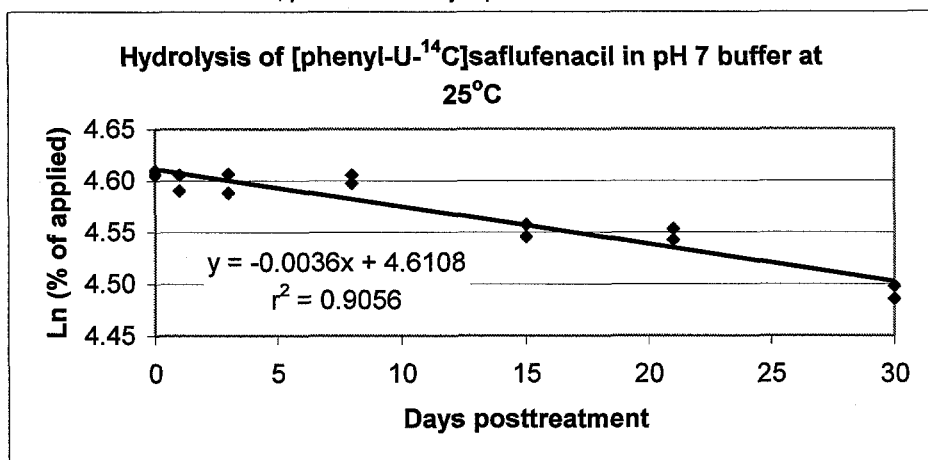
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.61743455	0.008854391	521.4853	1.66E-27	4.598142485	4.636726608	4.598142485	4.636726608
X Variable 1	-0.00196596	0.000578477	-3.39851	0.005284	-0.00322635	-0.000705569	-0.003226353	-0.000705569

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Phenyl Label at pH 7 Half-life: 192.54 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.4	4.6092
0	100.0	4.6052
1	98.5	4.5901
1	100.0	4.6052
3	100.1	4.6062
3	98.3	4.5880
8	99.2	4.5971
8	100.0	4.6052
15	95.3	4.5570
15	94.2	4.5454
21	94.9	4.5528
21	93.9	4.5422
30	88.7	4.4853
30	89.8	4.4976

Data obtained from Table 6, p. 40 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.95162533
R Square	0.90559076
Adjusted R Square	0.89772333
Standard Error	0.01323863
Observations	14

ANOVA

	df	SS	MS	F	Significance F
Regression	1	0.020173674	0.020174	115.1062	1.66628E-07
Residual	12	0.002103137	0.000175		
Total	13	0.02227681			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.61076547	0.005160765	893.4268	2.6E-30	4.599521131	4.622009813	4.599521131	4.622009813
X Variable 1	-0.00361735	0.000337164	-10.7288	1.67E-07	-0.00435197	-0.002882733	-0.004351967	-0.002882733

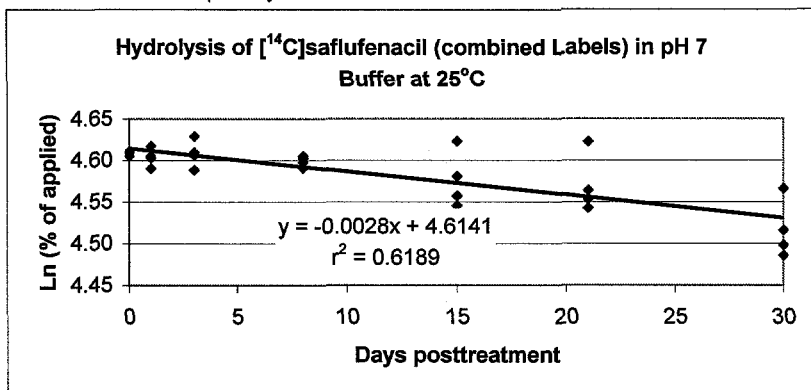
Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Combined Labels at pH 7 Half-life: 247.55 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.0	4.6052
0	100.6	4.6110
0	100.4	4.6092
0	100.0	4.6052
1	99.8	4.6029
1	101.2	4.6170
1	98.5	4.5901
1	100.0	4.6052
3	102.4	4.6289
3	100.4	4.6094
3	100.1	4.6062
3	98.3	4.5880
8	98.5	4.5903
8	99.7	4.6024
8	99.2	4.5971
8	100.0	4.6052
15	101.8	4.6227
15	97.6	4.5806
15	95.3	4.5570
15	94.2	4.5454
21	101.7	4.6221
21	95.9	4.5635
21	94.9	4.5528
21	93.9	4.5422
30	91.5	4.5159
30	96.1	4.5657
30	88.7	4.4853
30	89.8	4.4976

Data obtained from Table 6, p. 40 and Table 12, p. 46 of the study report.

Data reported to one decimal in the phenyl label, and to two decimals in the uracil label; all data was rounded to one decimal place by the reviewer.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.78671391
R Square	0.61891877
Adjusted R Square	0.6042618
Standard Error	0.02385525
Observations	28

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	0.024030208	0.02403	42.22692	6.89577E-07
Residual	26	0.014795902	0.000569		
Total	27	0.03882611			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.61410001	0.00657567	701.6928	3.84E-57	4.600583527	4.627616492	4.600583527	4.627616492
X Variable 1	-0.00279166	0.000429603	-6.49822	6.9E-07	-0.003674717	-0.001908594	-0.003674717	-0.001908594

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

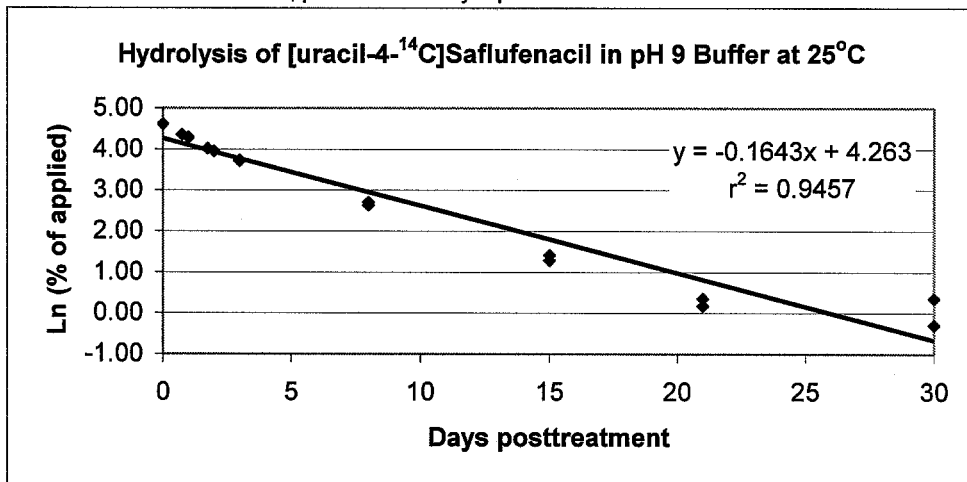
Uracil Label at pH 9

Half-life:

4.22 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.10	4.6062
0	100.00	4.6052
0.75	77.72	4.3531
1	72.84	4.2883
1	71.74	4.2730
1.75	55.39	4.0144
2	51.86	3.9485
3	41.86	3.7343
3	40.89	3.7109
8	13.87	2.6297
8	14.88	2.7000
15	4.08	1.4061
15	3.59	1.2782
21	1.41	0.3436
21	1.18	0.1655
30	1.42	0.3507
30	0.74	-0.3011

Data obtained from Table 14, p. 48 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.97246087
R Square	0.94568014
Adjusted R Square	0.94205881
Standard Error	0.42794516
Observations	17

ANOVA

	df	SS	MS	F	Significance F
Regression	1	47.8247913	47.82479	261.1421	6.7534E-11
Residual	15	2.747055865	0.183137		
Total	16	50.57184716			

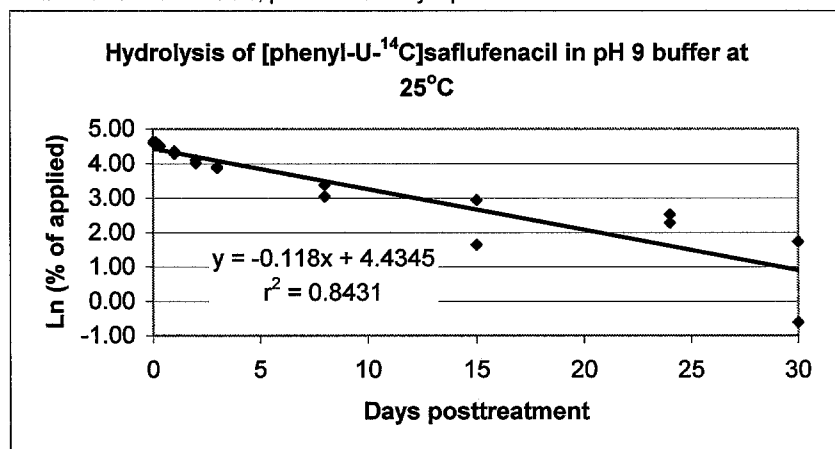
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.26304559	0.141362492	30.15684	7.7E-15	3.961738576	4.564352611	3.961738576	4.564352611
X Variable 1	-0.1642691	0.010165237	-16.1599	6.75E-11	-0.185935814	-0.142602434	-0.185935814	-0.142602434

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Phenyl Label at pH 9 Half-life: 5.87 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.0	4.6052
0	99.51	4.6003
0.12	100.10	4.6062
0.17	96.95	4.5742
0.17	94.57	4.5493
0.25	93.97	4.5430
0.33	89.71	4.4966
0.33	88.48	4.4828
1	77.62	4.3518
1	71.57	4.2707
2	54.64	4.0008
2	60.38	4.1007
3	48.88	3.8894
3	47.50	3.8607
8	29.08	3.3701
8	20.90	3.0397
15	18.83	2.9355
15	5.12	1.6332
24	12.37	2.5153
24	9.75	2.2773
30	5.60	1.7228
30	0.54	-0.6162

Data obtained from Table 8, p. 42 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.91822368
R Square	0.84313473
Adjusted R Square	0.83529146
Standard Error	0.54405855
Observations	22

ANOVA					
	df	SS	MS	F	Significance F
Regression	1	31.81936071	31.81936	107.4979	1.71677E-09
Residual	20	5.919994213	0.296		
Total	21	37.73935492			

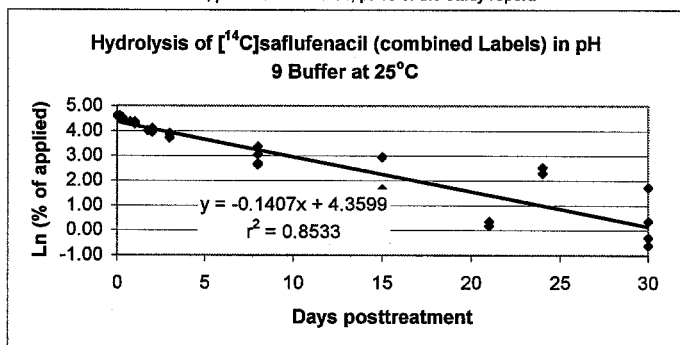
	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.43451875	0.144747543	30.63623	2.78E-18	4.132580665	4.736456831	4.132580665	4.736456831
X Variable 1	-0.1180044	0.011381462	-10.3681	1.72E-09	-0.141745697	-0.094263069	-0.141745697	-0.094263069

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Combined Labels at pH 9 Half-life: 4.93 days

Days Posttreatment	Saflufenacil	
	% of applied	Ln (% of applied)
0	100.10	4.6062
0	100.00	4.6052
0	100.0	4.6052
0	99.51	4.6003
0.12	100.10	4.6062
0.17	96.95	4.5742
0.17	94.57	4.5493
0.25	93.97	4.5430
0.33	89.71	4.4966
0.33	88.48	4.4828
0.75	77.72	4.3531
1	72.84	4.2883
1	71.74	4.2730
1	77.62	4.3518
1	71.57	4.2707
1.75	55.39	4.0144
2	51.86	3.9485
2	54.64	4.0008
2	60.38	4.1007
3	41.86	3.7343
3	40.89	3.7109
3	48.88	3.8894
3	47.50	3.8607
8	13.87	2.6297
8	14.88	2.7000
8	29.08	3.3701
8	20.90	3.0397
15	4.08	1.4061
15	3.59	1.2782
15	18.83	2.9355
15	5.12	1.6332
21	1.41	0.3436
21	1.18	0.1655
24	12.37	2.5153
24	9.75	2.2773
30	1.42	0.3507
30	0.74	-0.3011
30	5.60	1.7228
30	0.54	-0.6162

Data obtained from Table 8, p. 42 and Table 14, p. 48 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.92376554
R Square	0.85334277
Adjusted R Square	0.84937906
Standard Error	0.61309655
Observations	39

ANOVA

	df	SS	MS	F	Significance F
Regression	1	80.92440491	80.9244	215.289	5.29741E-17
Residual	37	13.90783316	0.375887		
Total	38	94.83223807			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	4.35991914	0.127020528	34.32452	1.17E-29	4.102551113	4.617287175	4.102551113	4.617287175
X Variable 1	-0.14066931	0.009587127	-14.67273	5.3E-17	-0.160094675	-0.121243947	-0.160094675	-0.121243947

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

3- to 24-day
Half-life:

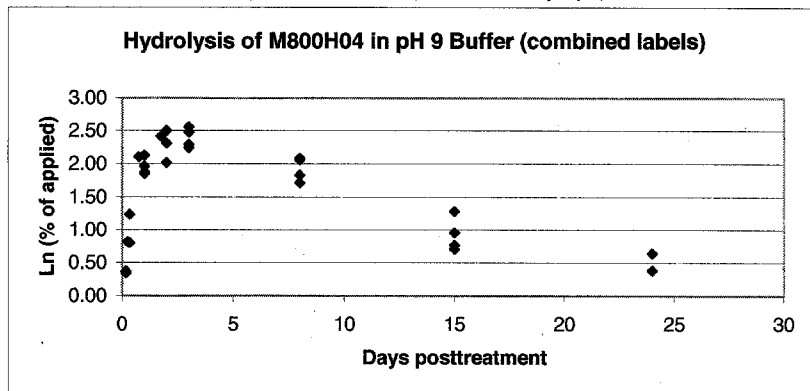
7.04 days

M800H04

Combined Labels in pH 9

Days	M800H04	
Posttreatment	% of applied	Ln (% of applied)
0.17	1.41	0.3436
0.17	1.45	0.3716
0.25	2.26	0.8154
0.33	2.23	0.8020
0.33	3.42	1.2296
0.75	8.19	2.1029
1	7.12	1.9629
1	8.39	2.1270
1	6.36	1.8500
1	6.54	1.8779
1.75	11.18	2.4141
2	12.21	2.5023
2	10.11	2.3135
2	7.51	2.0162
3	12.89	2.5565
3	11.90	2.4765
3	9.92	2.2946
3	9.40	2.2407
8	7.85	2.0605
8	8.04	2.0844
8	5.56	1.7156
8	6.25	1.8326
15	2.02	0.7031
15	2.15	0.7655
15	3.59	1.2782
15	2.60	0.9555
24	1.47	0.3853
24	1.90	0.6419

Data obtained from Table 8, p. 42 and Table 14, p. 48 of the study report.



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.94772413
R Square	0.89818103
Adjusted R Square	0.88969612
Standard Error	0.25212433
Observations	14

ANOVA

	df	SS	MS	F	Significance F
Regression	1	6.728929379	6.728929	105.8562	2.63114E-07
Residual	12	0.76280016	0.063567		
Total	13	7.491729539			

	Coefficients	Standard Error	t Stat	P-value	Lower 95%	Upper 95%	Lower 95.0%	Upper 95.0%
Intercept	2.64006242	0.123862326	21.31449	6.63E-11	2.370189591	2.909935241	2.370189591	2.909935241
X Variable 1	-0.09848785	0.00957248	-10.28865	2.63E-07	-0.119344493	-0.07763121	-0.119344493	-0.077631211

Chemical: Saflufenacil
 MRID: 47127823
 PC Code: 118203
 Guideline: 835.2120

Uracil Label

pH 5

Days posttreatment	% applied radioactivity			Days posttreatment	% applied radioactivity		
	Total	Average	SD		Total	Average	SD
0	101.5	100.8	1.1	0	100.0	100.3	0.4
0	100.0			0	100.6		
1	101.9	101.1	1.2	1	99.8	100.5	1.0
1	100.2			1	101.2		
3	101.8	102.2	0.6	3	102.4	101.4	1.4
3	102.6			3	100.4		
8	103.0	103.9	1.2	8	101.2	101.9	0.9
8	104.7			8	102.5		
15	102.4	102.2	0.3	15	106.2	103.8	3.5
15	102.0			15	101.3		
21	102.7	102.5	0.4	21	106.5	104.4	3.0
21	102.2			21	102.2		
30	103.1	102.2	1.3	30	99.9	101.0	1.5
30	101.3			30	102.0		
Total		102.1	1.2	Total		101.9	2.1

pH 9

Days posttreatment	% applied radioactivity		
	Total	Average	SD
0	100.1	100.1	0.1
0	100.0		
0.75	99.5		
1	97.0	96.9	0.1
1	96.8		
1.75	98.4		
2	97.9		
3	100	98.7	1.9
3	97.3		
8	96.5	96.7	0.2
8	96.8		
15	96.9	96.8	0.1
15	96.7		
21	94.8	96.6	2.5
21	98.3		
30	95.8	96.6	1.1
30	97.4		
Total		97.7	1.5

Data obtained from Table 3, p. 37 of the study report.
 Single samples collected at 0.75, 1.75, and 2 days posttreatment.

Chemical: Saflufenacil
 MRID: 47127823
 PC Code: 118203
 Guideline: 835.2120

Phenyl Label

pH 5

Days posttreatment	% applied radioactivity			Days posttreatment	% applied radioactivity		
	Total	Average	SD		Total	Average	SD
0	100.1	100.1	0.1	0	100.4	100.2	0.3
0	100.0			0	100.0		
1	100.4	99.5	1.3	1	99.4	99.7	0.4
1	98.6			1	100.0		
3	99.6	99.7	0.1	3	100.1	99.2	1.3
3	99.8			3	98.3		
8	99.9	100.4	0.7	8	101.6	101.9	0.4
8	100.9			8	102.1		
15	100.2	100.5	0.4	15	102.0	100.6	2.1
15	100.7			15	99.1		
21	99	100.4	2.0	21	101.4	101.2	0.3
21	101.8			21	101.0		
30	101.4	100.8	0.9	30	100.5	100.3	0.3
30	100.1			30	100.1		
Total		100.2	0.9	Total		100.4	1.1

pH 9

Days posttreatment	% applied radioactivity		
	Total	Average	SD
0	100.0	99.8	0.4
0	99.5		
0.12	100.1		
0.17	101.0	100.4	0.9
0.17	99.7		
0.25	100.4		
0.33	99.9	99.8	0.2
0.33	99.6		
1	101.3	100.5	1.2
1	99.6		
2	100.0	100.0	0.0
2	100.0		
3	100.0	99.6	0.6
3	99.2		
8	100.0	100.2	0.2
8	100.3		
15	102.1	100.3	2.5
15	98.5		
24	106.3	103.8	3.6
24	101.2		
30	104.4	102.2	3.2
30	99.9		
Total		100.6	1.7

Data obtained from Table 3, p. 37 of the study report; single samples collected at 0.12 and 0.25 days.

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Uracil Label at pH 5

Days posttreatment	% applied radioactivity			% applied radioactivity		
	Parent	Average	SD	Trifluoroacetone	Average	SD
0	101.5	100.8	1.1	--		
0	100.0			--		
1	101.9	101.1	1.2	--		
1	100.2			--		
3	101.8	102.2	0.6	--		
3	102.6			--		
8	102.3	102.8	0.6	--		
8	103.2			--		
15	102.0	101.4	0.8	--		
15	100.8			--		
21	101.6	101.7	0.1	--		
21	101.8			--		
30	101.5	101.1	0.6	--		
30	100.6			--		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	Unk 16.2	Average	SD	M800H15	Average	SD	M800H04	Average	SD
0	--			--					
0	--			--					
1	--			--					
1	--			--					
3	--			--					
3	--			--					
8		0.7	0.6	0.2	--				
8		0.5			--		0.7		
15		0.5	0.3	0.2	--				
15		0.2			--		0.6		
21		0.9			--				
21					--		--		
30		0.5	0.3	0.2			0.5	0.4	0.2
30		0.2			0.2		0.2		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	Unk 18.5-18.6	Average	SD	Unk 20.8	Average	SD	Other	Average	SD
0	--			--			--		
0	--			--			--		
1	--			--			--		
1	--			--			--		
3	--			--			--		
3	--			--			--		
8	--						--		
8	--			0.4			--		
15	--						--		
15	--			0.4			--		
21	--			--			0.2		
21	--			--					
30		0.2			0.3		0.2		
30									

Data obtained from Table 10, p. 44 of the study report.

— Blank cells were presented in the table, with no indication of what they represented.

Study authors presented data to one and two decimal places.

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Uracil Label at pH 7

Days posttreatment	% applied radioactivity			% applied radioactivity		
	Parent	Average	SD	Trifluoroacetone	Average	SD
0	100.00	100.3	0.4	--		
0	100.58			--		
1	99.77	100.5	1.0	--		
1	101.19			--		
3	102.40	101.4	1.4	--		
3	100.42			--		
8	98.52	99.1	0.8	0.97	1.4	0.6
8	99.72			1.81		
15	101.77	99.7	3.0	2.35	2.4	0.1
15	97.57			2.49		
21	101.71	98.8	4.1	3.66	4.1	0.6
21	95.92			4.54		
30	91.46	93.8	3.3	4.73	4.5	0.3
30	96.13			4.35		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	Unk 16.2	Average	SD	M800H15	Average	SD	M800H04	Average	SD
0	--			--			--		
0	--			--			--		
1	--			--			--		
1	--			--			--		
3	--			--			--		
3	--			--			--		
8	0.75	0.80	0.1	0.54			0.23		
8	0.84								
15	0.42	0.39	0.0	0.81	0.7	0.1	0.87	0.56	0.4
15	0.35			0.68			0.24		
21				0.86	0.8	0.1	0.24	0.2	0.0
21	0.71			0.75			0.24		
30	0.79			1.82	1.7	0.2	0.95		
30				1.53					

Days posttreatment	% applied radioactivity		
	Unk 20.8	Average	SD
0	--		
0	--		
1	--		
1	--		
3	--		
3	--		
8	0.19	0.2	0.0
8	0.14		
15	--		
15	--		
21	--		
21	--		
30	0.14		
30			

Data obtained from Table 12, p. 46 of the study report.

-- Blank cells were presented in the table, with no indication of what they represented.

Chemical: Saffluenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Uracil Label at pH 9

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	Parent	Average	SD	Trifluoroacetone	Average	SD	Unknown 6.4	Average	SD
0	100.10	100.1	0.1	--			--		
0	100.00			--			--		
0.75	77.72			8.24			--		
1	72.84	72.3	0.8	10.59	10.7	0.1	--		
1	71.74			10.71			--		
1.75	55.39			21.92			--		
2	51.86			25.81			--		
3	41.86	41.4	0.7	34.17	32.4	2.5	--		
3	40.89			30.68			--	4.87	
8	13.87	14.4	0.7	57.01	56.8	0.4	--		
8	14.88			56.49			--		
15	4.08	3.8	0.3	69.27	68.7	0.7	--		
15	3.59			68.21			--		
21	1.41	1.3	0.2	70.51	72.2	2.5	--		
21	1.18			73.98			--		
30	1.42	1.1	0.5	70.16	71.7	2.1	--		
30	0.74			73.20			--		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	M800H15	Average	SD	M800H04	Average	SD	Unk18.5-18.6	Average	SD
0	--			--			--		
0	--			--			--		
0.75	1.77			8.19			1.95		
1	2.46	2.6	0.2	7.12	7.8	0.9	2.95	2.8	0.3
1	2.75			8.39			2.55		
1.75	4.47			11.18			1.46		
2	4.53			12.21			1.39		
3	6.56	6.2	0.5	12.89	12.4	0.7	1.76	1.4	0.6
3	5.86			11.90			0.96		
8	14.40	14.0	0.5	7.85	7.9	0.1	1.01	0.9	0.1
8	13.68			8.04			0.82		
15	19.10	19.3	0.3	2.02	2.1	0.1	--		
15	19.48			2.15			--		
21	21.75	21.7	0.0	--			--		
21	21.71			--			--		
30	21.60	21.8	0.3	--			--		
30	22.09			--			--		

Days posttreatment	% applied radioactivity			% applied radioactivity		
	Unk 20.1	Average	SD	Other	Average	SD
0	--			--		
0	--			--		
0.75	1.61			--		
1	1.04	0.9	0.2	--		
1	0.70			--		
1.75	3.95			--		
2	2.15			--		
3	2.74	2.5	0.4	--		
3	2.17			--		
8	2.39	2.6	0.3	--		
8	2.88			--		
15	1.44	1.6	0.3	--		
15	1.81			--		
21	0.32	0.6	0.4	--		
21	0.83			--		
30	0.39			--		
30				--		

Data obtained from Table 14, p. 48 of the study report.

-- Blank cells were presented in the table, with no indication of what they represented.

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Phenyl Label pH 5

Days posttreatment	% applied radioactivity			% applied radioactivity		
	Parent	Average	SD	Unk 24.0	Average	SD
0	100.1	100.1	0.1	--		
0	100.0			--		
1	100.4	99.5	1.3	--		
1	98.6			--		
3	99.6	99.7	0.1	--		
3	99.8			--		
8	99.9	100.4	0.7	--		
8	100.9			--		
15	98.9	99.6	0.9	0.80	0.7	0.2
15	100.2			0.52		
21	99.0	100.4	2.0	--		
21	101.8			--		
30	101.4	100.8	0.9	--		
30	100.1			--		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity	
	M800H07	Average	SD	Unk 26.8	Average	SD	M800H15	SD
0	--			--			--	
0	--			--			--	
1	--			--			--	
1	--			--			--	
3	--			--			--	
3	--			--			--	
8	--			--			--	
8	--			--			--	
15	--			0.39			0.16	
15	--							
21	--			--			--	
21	--			--			--	
30	--			--			--	
30	--			--			--	

Data obtained from Table 5, p. 39 of the study report.

-- Blank cells were presented in the table, with no indication of what they represented.
 Study authors presented data to one and two decimal places.

Chemical: Saflufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Phenyl Label pH 7

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	Parent	Average	SD	Unk 24.0	Average	SD	M800H07	Average	SD
0	100.4	100.2	0.3	--			--		
0	100.0			--			--		
1	98.5	99.3	1.1	--			--		
1	100.0			--			--		
3	100.1	99.2	1.3	--			--		
3	98.3			--			--		
8	99.2	99.6	0.6	--			1.9	1.8	0.2
8	100.0			--			1.6		
15	95.3	94.8	0.8	0.7			4.1	3.8	0.5
15	94.2						3.4		
21	94.9	94.4	0.7	--			4.9	5.3	0.6
21	93.9			--			5.7		
30	88.7	89.3	0.8	--			9.2	8.6	0.8
30	89.8			--			8.0		

Days posttreatment	% applied radioactivity			% applied radioactivity			% applied radioactivity		
	M800H15	Average	SD	M800H04	Average	SD	Unk 39.3	Average	SD
0	--			--			--		
0	--			--			--		
1	--			--			0.9		
1	--			--			--		
3	--			--			--		
3	--			--			--		
8	0.2	0.2	0.0	0.4	0.3	0.1	--		
8	0.2			0.2			--		
15	1.4	1.2	0.3	0.6	0.6	0.1	--		
15	1.0			0.5			--		
21	1.66	1.5	0.2	--			--		
21	1.4			--			--		
30	1.8	2.1	0.4	0.7			--		
30	2.3						--		

Data obtained from Table 6, p. 40 of the study report.

-- Blank cells were presented in the table, with no indication of what they represented.
Study authors presented data to one and two decimal places.

Chemical: Salfufenacil
MRID: 47127823
PC Code: 118203
Guideline: 835.2120

Phenyl Label at pH 9

Days posttreatment	% applied radioactivity				% applied radioactivity				% applied radioactivity			
	Parent	Average	SD		M800H07	Average	SD		M800H15	Average	SD	
0	100.0	99.8	0.3		--				--			
0	99.51				--				--			
0.12	100.10				--				--			
0.17	96.95	95.8	1.7		0.81	0.9	0.2		--			
0.17	94.57				1.04				0.84			
0.25	93.97				1.64				1.09			
0.33	89.71	89.1	0.9		2.49	2.4	0.2		2.10	2.1	0.1	
0.33	88.48				2.22				2.18			
1	77.62	74.6	4.3		11.69	12.3	0.8		3.63	3.8	0.3	
1	71.57				12.89				4.00			
2	54.64	57.5	4.1		24.78	23.8	1.3		8.76	7.6	1.7	
2	60.38				22.89				6.35			
3	48.88	48.2	1.0		32.11	32.5	0.5		9.11	9.0	0.1	
3	47.50				32.82				8.98			
8	29.08	25.0	5.8		50.19	53.5	4.6		15.21	15.8	0.8	
8	20.90				56.75				16.37			
15	18.83	12.0	9.7		63.32	66.5	4.5		16.34	18.3	2.8	
15	5.12				69.71				20.29			
24	12.37	11.1	1.9		71.35	70.0	2.0		20.22	20.1	0.2	
24	9.75				68.58				19.89			
30	5.60	3.1	3.6		76.40	76.7	0.4		21.08	21.3	0.3	
30	0.54				76.92				21.54			

Days posttreatment	% applied radioactivity				% applied radioactivity				% applied radioactivity			
	M800H04	Average	SD		Unk 29.3	Average	SD		Unk 29.8	Average	SD	
0	--				--				--			
0	--				--				--			
0.12	--				--				--			
0.17	1.41	1.4	0.0		--				1.83	1.5	0.4	
0.17	1.45				0.6				1.23			
0.25	2.26				1.5				--			
0.33	2.23	2.8	0.8		0.6	0.8	0.2		2.28	2.1	0.3	
0.33	3.42				0.9				1.85			
1	6.36	6.5	0.1		0.6	0.9	0.3		1.37	1.9	0.8	
1	6.54				1.1				2.49			
2	10.11	8.8	1.8		0.5	0.6	0.2		1.18	1.7	0.7	
2	7.51				0.7				2.17			
3	9.92	9.7	0.4		--							
3	9.40				--				0.46			
8	5.56	5.9	0.5		--				--			
8	6.25				--				--			
15	3.59	3.1	0.7		--				--			
15	2.60				--				--			
24	1.47	1.7	0.3		--				--			
24	1.90				--				--			
30					--				--			
30					--				--			

Days posttreatment	% applied radioactivity			
	Other	Average	SD	
0	--			
0	--			
0.12	--			
0.17	--			
0.17	--			
0.25	--			
0.33	0.50	0.5	0.0	
0.33	0.52			
1	--			
1	1.03			
2	--			
2	--			
3	--			
3	--			
8	--			
8	--			
15	0.73			
15	--			
24	0.86	1.0	0.2	
24	1.10			
30	1.34	1.1	0.3	
30	0.93			

Data obtained from Table 8, p. 42 of the study report.

-- Blank cells were presented in the table, with no indication of what they represented.

Attachment 3: Transformation Pathway Presented by Registrant

FIGURE 6. DEGRADATION PATHWAY ON HYDOLYSIS OF BAS 800 IN NEUTRAL OR BASIC WATER

